



chain nodes :

37 38 39 40 41 42 44 45 47 48 50 51 52 53 55 56 57 58
60 64 65

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
22 23 24 25 26 27 28 29 30 31 32 33 34 35 36

ring/chain nodes :

59

chain bonds :

5-37 7-64 9-37 11-38 14-38 17-39 18-50 19-41 22-40 23-55 25-65
27-41 29-42 32-42 37-44 38-45 39-40 41-47 42-48 50-51 50-52
50-53 55-56 55-57 55-58

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14
13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23
23-24 25-26 25-30 26-27 27-28 28-29 29-30 31-32 31-36 32-33
33-34 34-35 35-36

exact/norm bonds :

5-37 7-64 9-37 11-38 14-38 18-50 19-41 23-55 25-65 27-41 29-42
32-42 37-44 38-45 41-47 42-48 50-51 50-52 50-53 55-56 55-57
55-58

exact bonds :

17-39 22-40 39-40

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14
13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23
23-24 25-26 25-30 26-27 27-28 28-29 29-30 31-32 31-36 32-33
33-34 34-35 35-36

isolated ring systems :

containing 1 : 13 : 1 25 : 31 :

G1:H,CH3

G2:[*1],[*2]

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom	
18:Atom	19:Atom	20:Atom	21:Atom	22:Atom	23:Atom	24:Atom	25:Atom	
26:Atom	27:Atom	28:Atom	29:Atom	30:Atom	31:Atom	32:Atom	33:Atom	
34:Atom	35:Atom	36:Atom	37:CLASS	38:CLASS	39:CLASS	40:CLASS		
41:CLASS	42:CLASS	44:CLASS	45:CLASS	47:CLASS	48:CLASS	50:CLASS		
51:CLASS	52:CLASS	53:CLASS	55:CLASS	56:CLASS	57:CLASS	58:CLASS		
59:CLASS	60:CLASS	64:CLASS	65:CLASS					